

lonization Polarity Prediction of Compounds for Efficient Mass Spectrometry James Francis Blake et al. 09/898,290

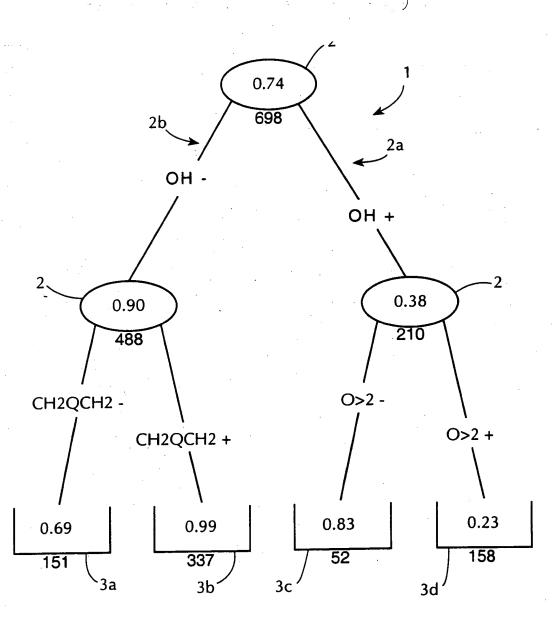


Figure 1



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- a) s I cting a data base of a statistically signifi ant group f compounds and determining the p larization,
 p sitiv r negative, at which each of aid compound is ionized;
- b) structurally analyzing the individual compounds to determine structural characteristics common to a majority of compounds which ionize at positive polarity and to determine structural characteristics common to a majority of compounds which ionize at negative polarity, as polarization determinants;
- c) sequentially arranging the polarization determinants in classification trees according to percentage determination of one of said negative or positive polarization:
- d) applying the polarization determinants in one of said classification trees in classifying a new compound for a predicted polarization of positive or negative at which said compound is ionized;
- e) segregating compounds classified as ionizing at positive polarity and compounds classified as ionizing at negative polarity; and
- f) separately analyzing the segregated compounds with the respective predicted polarities with an